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Stochastic Models for Many-Body Systems

I. Infinite Systems in Thermal Equilibrium

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STOCHASTIC MODELS FOR MANY-BODY SYSTEMS
I. INFINITE SYSTEMS IN THERMAL EQUILIBRIUM

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ABSTRACT

Some model Hamiltonians are proposed for quantum-mechanical many-body systems with pair forces. In the case of an infinite system in thermal equilibrium, they lead to temperature-domain propagator expansions which are expressible by closed, formally exact equations. The expansions are identical with infinite subclasses of terms from the propagator expansion for the true many-body problem. The two principal models introduced correspond, respectively, to ring and ladder summations from the true propagator expansion, but augmented by infinite classes of self-energy corrections. The latter are expected to yield damping of single-particle excitations. The eigenvalues of the ring and ladder model Hamiltonians are real, and they are bounded from below if the pair potential obeys certain conditions. The models are formulated for fermions, bosons, and distinguishable particles. In addition to the ring and ladder models, two simpler types are discussed, one of which yields the Hartree-Fock approximation to the true problem. A novel feature of all the model Hamiltonians (except the Hartree-Fock) is that they contain an infinite number of parameters whose phases are fixed by random choices. Explicit closed expressions are obtained for the Helmholtz free energy of all the models in the classical limit.

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1. INTRODUCTION

A difficulty in calculating the statistical behavior of many-body systems is that some quantities of interest may not have convergent perturbation expansions. If the system is infinite in size, this can occur even when the density of particles is very low and the interparticle forces are very weak. The situation is already present in the classical theory. Consider a gas of classical particles which interact by a repulsive, short-range pair-potential $\lambda V(x)$. If the pressure, expressed as a function of density and temperature, is expanded in powers of the strength parameter λ , the expansion has zero radius of convergence.¹ This suggests that a similar situation may exist in the quantum-mechanical case.

Non-convergence of interaction-strength expansions is not necessarily a disaster. In the classical example just cited, the expansion almost certainly is asymptotic about $\lambda = 0$, and we may hope that this is true also in some quantum-mechanical cases. However, many physical problems of interest do not exhibit weak interactions. Moreover, certain properties of a quantum-mechanical many-body system may not have even asymptotic expansions as power-series in λ . An example is the one-particle momentum distribution $\sigma(k)$ [normalization: $\int \sigma(k) d^3k = 1$]. For an infinite system, a finite change in $\sigma(k)$ from its form for uncoupled particles means that an infinite number of particles are displaced from the momentum levels they would occupy if they were not coupled. In order to form such a state from the uncoupled state, the interaction Hamiltonian must act an infinite number of times; that is, infinite orders of perturbation theory are involved. We expect on physical grounds that the change in $\sigma(k)$ goes to

zero as λ does. However, we cannot presume that it must go to zero as some integral power of λ .

In recent years, several formalisms for handling perturbation expansions in the quantum-mechanical many-body problem have been proposed which are related to methods previously used in quantum electrodynamics.²⁻¹⁰ They produce great simplifications in manipulations and permit one to carry out various formal summations of infinite classes of terms from the perturbation expansions. These formalisms are a natural choice for investigating quantities, such as $\sigma(k)$, which may not have convergent or asymptotic expansions. However, it can be difficult to know in advance what summations should be carried out in given cases. With sufficient ingenuity, it is possible to sum certain divergent series so as to obtain almost any answer whatever. It is difficult to guess in advance whether adding further infinite classes of terms to a known expansion will improve the answer or make it worse.

In the present paper we shall describe a procedure intended to pick out perturbation-term summations for which certain characteristics are predictable in advance. We shall formulate model Hamiltonians such that the complete perturbation expansions to which they lead are formally identical with certain infinite subclasses of terms from the corresponding perturbation expansion for the true Hamiltonian. The model Hamiltonians are Hermitian, and have eigenvalues which are bounded from below if the pair potential obeys certain restrictions. The predictable characteristics of the model solutions are those which follow from these properties.

In common with the true many-body Hamiltonian, our models (with one exception) are not diagonalizable by known means. However, they are soluble in the sense that they yield formally closed integral equations for the propagators that determine the mean energies, mean occupation numbers, etc. which are of statistical-mechanical interest. A novel feature of the models is that they contain infinite numbers of parameters whose values are chosen at random. We shall therefore call them stochastic models. The random parameters will be described in Secs. 2 and 3.

We shall present two principal types of stochastic models, ladder and ring. They correspond, respectively, to summations of familiar infinite classes of ladder or ring diagrams from the perturbation series for the true Hamiltonian. At the same time, however, they include certain infinite classes of self-energy corrections to these diagrams. The corrections are of a type expected to contribute to the damping of elementary excitations. In addition to the ladder and ring models, we shall introduce two simpler types. One yields the Hartree-Fock approximation to the true problem (and contains no random parameters). The other also includes the Hartree-Fock diagrams, but with iterated self-energy corrections. The eigenvalues of this last model are not bounded from below for any pair potential, and its validity therefore is quite doubtful.

The models which are described in the present paper yield closed equations only for infinite systems. We shall develop each type of model in two forms: for indistinguishable particles (fermions and bosons) and for distinguishable particles. The analytical treatment will begin with the distinguishable particle models. They admit more immediate physical interpretations. We shall apply to them the Ursell-Mayer irreducible

cluster expansion method and thereby obtain an explicit closed expression for the Helmholtz free energy of each model in the classical limit. For the fermion and boson models, we shall use a temperature-domain propagator formalism of the type originated by Matsubara² and developed further by Fradkin,⁵ Abrikosov et al.,⁶ Luttinger and Ward,⁸ and others. The distinguishable and indistinguishable particle models turn out to give formally identical thermodynamics in the classical limit. Thus, our classical results for the Helmholtz free energy provide some insights into the behavior of the fermion and boson models.

In the paper which follows, we develop more general models which yield closed equations whatever the size of the system.¹¹ We shall apply them to non-equilibrium as well as equilibrium statistical mechanics. For an infinite system in equilibrium, the generalized models yield the same final equations as the models of the present paper. However, they provide a neater and more satisfactory derivation of these equations. We do not start with the general treatment in the present paper because it requires a more elaborate formalism and therefore does not provide as direct an introduction to the use of stochastic models.

The derivation of our closed model equations involves a deep-lying convergence question which is described in Sec. 5.1. We make no attempt to answer this question in the present paper. In the following paper, we offer what we hope is a satisfying, although non-rigorous, resolution.

2. MODELS FOR DISTINGUISHABLE PARTICLES

2.1 Nature of the Models

Let us consider a system of N similar but distinguishable particles (of unit mass) which interact through a pair potential $V(x)$. The total Hamiltonian may be written

$$H = \frac{1}{2} \sum_n p_n^2 + \frac{1}{2} \sum_{n,m}' V(x_n - x_m) \quad (n, m = 1, 2, \dots, N), \quad (2.1)$$

where \sum' means that $n = m$ is omitted in the sum. Here p_n and x_n are the momentum and position of the n th particle. We shall adopt the artifice of confining the system in a cubical cyclic box of volume Ω . That is, we restrict $V(x)$ to the form

$$V(x) = \sum_k V_k \exp(ik \cdot x), \quad (2.2)$$

where k takes all the values allowed by cyclic boundary conditions on the walls of the box, and we require that the Schrödinger wave function be a cyclic function of the coordinates of each particle. In the classical case, we assume that a particle which exits through any wall of the box simultaneously re-enters, with the same momentum, through the opposite wall. We shall eventually be interested in the limit $N \rightarrow \infty$, $\Omega \rightarrow \infty$, with N/Ω finite.

We require that $V(x)$ be real and have reflectional symmetry. These conditions imply

$$V(x) = V(-x), \quad V_k = V_{-k}, \quad V_k = V_k^*. \quad (2.3)$$

Except where we specify otherwise, we shall assume that $V(x)$ is a smooth, bounded function such that

$$|V_k| = O(\Omega^{-1}), \quad \Omega \rightarrow \infty \text{ (all } k),$$

$$|V_k| \leq O(k^{-2}), \quad k \rightarrow \infty.$$

In particular, this implies that $\int V(x) d^3x$ and $\int [V(x)]^2 d^3x$ exist for $\Omega \rightarrow \infty$, where the integration is over the whole box.

We shall call (2.1) the true Hamiltonian, and refer to the statistical-mechanical problem associated with it as the true problem.

Now let us consider model Hamiltonians of the form

$$H = \frac{1}{2} \sum_n p_n^2 + \frac{1}{2} \sum_{n,m} V^{n,m}(x_n - x_m), \quad (2.4)$$

where $V^{n,m}(x)$ is a pair potential which may be different for each pair of particles n and m . We require that $V^{n,m}(x)$ be real, and we replace (2.3) by

$$V^{n,m}(x) = V^{m,n}(-x). \quad (2.5)$$

Let us write

$$V^{n,m}(x) = \sum_k V_k^{n,m} \exp(ik \cdot x) \quad (2.6)$$

and define the parameters $\phi_{n,m;k}$ by

$$V_k^{n,m} = V_k \phi_{n,m;k} \quad (2.7)$$

Then the reality condition and (2.5) imply

$$\phi_{n,m;k} = \phi_{n,m;-k}^*, \quad \phi_{n,m;k} = \phi_{m,n;-k}. \quad (2.8)$$

The true problem, of course, corresponds to $\phi_{n,m;k} = 1$ for all n, m , and k . In the models with which we shall be concerned here, all the $\phi_{n,m;k}$ will be assigned unit modulus (except in the Hartree-Fock model where most of them will vanish). However, for each triad n, m, k the phase of $\phi_{n,m;k}$ will be assigned by a random choice, subject to (2.8) and to additional constraints which differ for each model. As we shall see, the models so produced have certain properties in common with the true Hamiltonian but lead to a statistical mechanics that can be expressed in closed form in the limit $\Omega \rightarrow \infty$.

2.2 Ladder Model

Let us specialize $\phi_{n,m;k}$ to the form

$$\phi_{n,m;k} = \exp(-ik \cdot d_{n,m}), \quad d_{n,m} = -d_{m,n}, \quad (2.9)$$

the $\wedge d_{n,m}$ are constant, real vectors. This clearly satisfies (2.8).

Now, for each pair n, m let us give the three vector-components of $d_{n,m}$ values chosen at random within the interval $(0, L)$ where $L = \Omega^{1/3}$. The choices are to be completely independent for pairs which are not identical. In the x representation, we have

$$V^{n,m}(x) = V(x - d_{n,m}), \quad (2.10)$$

which permits a very simple interpretation of this model: The pair potential has the same shape as in the true problem, but the particles now collide with ghosts of each other, displaced by the randomly chosen vectors $d_{n,m}$. For reasons which will appear later, we shall call this the ladder model.

An important feature of the ladder model is immediately apparent from (2.10). If $V(x)$ is non-negative for all x , then $V^{n,m}(x)$ also has this property. It follows that in this case the expectation of H in any quantum-mechanical state is non-negative, or, in other words, that all the eigenvalues of H are non-negative.

At this point, we want to make as clear as possible the precise sense in which our model is stochastic. The values of the $d_{n,m}$ are chosen at random [subject to (2.9)]. Once chosen, however, they are fixed, and we work thereafter with the definite Hamiltonian embodying these values. In particular, the same choice of the $d_{n,m}$ will be employed for every member of the canonical or grand canonical ensemble which we use in describing the statistical mechanics of the system. The principal deductions we shall make about the statistical mechanics of the model will be valid only for typical assignments of values for the $d_{n,m}$, a situation which is familiar in stochastic problems. [Thus $d_{n,m} = 0$ (all n, m) is a possible result of a random assignment of values, but it is not typical. The probability of this assignment vanishes with extreme rapidity as $N \rightarrow \infty$.] Instead of restricting ourselves to typical assignments, we could equivalently employ

A statistical distribution of assignments and make our deductions about averages over the distribution. Such a procedure would have some formal advantages, but we feel that the analysis will be clearer if we do not introduce this additional kind of average.

We wish now to investigate the equilibrium thermodynamics of our model in the classical limit. The virial expansion of the Helmholtz free energy per particle for the true problem may be written

$$A = A_0 - \beta^{-1} \sum_{\alpha=1}^{\infty} (\alpha + 1)^{-1} \rho^{\alpha} B_{\alpha}. \quad (2.11)$$

Here $A_0 = \beta^{-1} \left\{ \ln \left[\rho (2\pi\hbar^2\beta)^{3/2} \right] - 1 \right\}$ is the Helmholtz function for free particles, ρ is N/Ω , B_{α} is the Mayer irreducible cluster integral for a cluster of $\alpha + 1$ particles, and $\beta = 1/kT$, where k is Boltzmann's constant and T is absolute temperature. Equation (2.11) is formally exact in the limit $\Omega, N \rightarrow \infty$. In the true problem it makes no difference, of course, which of the N particles are assumed to be in the cluster for which B_{α} is calculated; the interaction of all pairs is identical. If the derivation is retraced with a model potential $V^{n,m}(x)$, it is found that (2.11) is still valid provided that B_{α} is reinterpreted in the following way: It is the average value of the cluster integral when the latter is calculated for all possible choices of the $\alpha + 1$ particles from among the N particles in the system.¹²

Let us write

$$f(x) = \exp[-\beta V(x)] - 1, \quad f^{n,m}(x) = \exp[-\beta V^{n,m}(x)] - 1. \quad (2.12)$$

Then the model cluster integral B_1 [Fig. 1a] is

$$B_1 = N^{-2} \Omega^{-1} \sum_{n,m} ' \iint f^{n,m}(x_n - x_m) d^3 x_n d^3 x_m, \quad (2.13)$$

where the integrations are over Ω , and we have replaced $N(N-1)$ by N^2 in anticipation of the limit $N \rightarrow \infty$. In the ladder model we have

$$f^{n,m}(x) = f(x - d_{n,m}).$$

Therefore, since $V(x)$ is cyclic, we find

$$B_1 = \int f(x) d^3 x, \quad (2.14)$$

which is identical with the result for the true problem.

Let us now assume that $V(x)$ has a finite range r_0 and is negligible for $|x| > r_0$. (Here x is measured modulo displacement by a cyclic period.) The next irreducible cluster integral [Fig. 1b] is

$$B_2 = N^{-3} \Omega^{-2} \sum_{n,m,\ell} ' \iiint f^{n,m}(x_n - x_m) f^{m,\ell}(x_m - x_\ell) \\ \times f^{\ell,n}(x_\ell - x_n) d^3 x_n d^3 x_m d^3 x_\ell. \quad (2.15)$$

Contributions to this integral can arise only from points which simultaneously satisfy

$$|x_n - x_m - d_{n,m}| \leq r_0, \quad |x_m - x_\ell - d_{m,\ell}| \leq r_0, \quad |x_\ell - x_n - d_{\ell,n}| \leq r_0. \quad (2.16)$$

However, since the $d_{n,m}$ have been fixed by random choices, and have values which range over the entire cyclic volume, it will be impossible to satisfy (2.16) for most triads n, m, ℓ . In fact, given a typical assignment of the d 's, it is clear that (2.16) can be satisfied only for a fraction of all triads which is of order r_0^3/Ω . It follows that B_2 vanishes as r_0^3/Ω in the limit $\Omega \rightarrow \infty, N \rightarrow \infty$. Similar considerations show that any given B_α ($\alpha > 1$) also vanishes in the limit. The contribution to B_α of each irreducible cluster diagram with $\alpha + 1$ particles and γ links vanishes as $(r_0^3/\Omega)^{\gamma-\alpha}$. Actually, the condition we placed on $V(x)$ is stronger than needed to obtain this result. It is sufficient that $f(x)$ be bounded and that $\int |f(x)| d^3x$ be finite in the limit.

On the basis of the preceding paragraph, let us assume that the total contribution to (2.11) from all B_α ($\alpha > 1$) vanishes in the limit. This is a non-trivial assumption. It involves a deep-lying convergence question which we shall discuss, in its quantum-mechanical form, in Sec. 5.1, and at length in the following paper. The essential point is that the number of irreducible diagrams of order α is enormous for $\alpha \sim O(N)$. For the present, we shall simply adopt the assumption. An equivalent assumption will be implicit in the discussion of the further classical models of Sec. 2. Retaining, then, only B_1 in the limit, we have

$$A - A_0 = \beta^{-1} a(\beta) \rho, \quad (2.17)$$

where $-2a(\beta)$ is the right side of (2.14). The corresponding equation of state is

$$p = \beta^{-1} \rho [1 + a(\beta) \rho], \quad (2.18)$$

where we define the pressure by the relation $p = \rho^{-2} (\partial A / \partial \rho) \beta$.

Equations (2.17) and (2.18) exhibit several properties of interest. First, we note that if $V(x)$ is non-negative everywhere, then $A - A_0$ is non-negative for all β and goes to zero as $\beta \rightarrow \infty$. This is consistent with our previous finding that the model potential energy is always non-negative for such $V(x)$.¹³ The present result provides some reassurance as to the validity of our formal procedures. A second property shows up most clearly if we take $V(x)$ to be a hard-sphere potential of range r_0 . Then we have $a(\beta) = \frac{2}{3} \pi r_0^3$. Now if we increase ρ without limit, we see that, in contrast to the true problem, the ladder model exhibits no saturation; the free energy and pressure continue to rise smoothly.¹⁴

A third fact of interest is that if $V(x)$ is negative anywhere, we have $\beta^{-1}a(\beta) \rightarrow -\infty$ as $\beta \rightarrow \infty$. Thus we have $A \rightarrow -\infty$ for any ρ , which indicates that there is no lower bound to the potential energy per particle. Furthermore, we have $(\partial p / \partial \rho)_\beta < 0$, for any given ρ , if the temperature is low enough. This suggests that the system then would be unstable to collapse, and, since there is no saturation, that the collapse would be catastrophic once it occurred.¹⁵ In the case of potentials with an attractive part, the ladder model offers the possibility of a valid approximation to the true problem only above a critical temperature for each ρ . It should be viewed with suspicion even above this temperature.

It is clear from (2.17) and (2.18) that the ladder model represents an extremely rudimentary approximation to the classical true problem. The interest of these results lies in the fact that they represent classical limits for the fermion and boson ladder models which

we shall introduce in Sec. 3. These models are non-trivial. A similar interest attaches to the further classical results to be presented in the remainder of Sec. 2.

2.3. Ring Model

Instead of adopting (2.9), let us now specialize $\phi_{n,m;k}$ to the form

$$\phi_{n,m;k} = \exp \left[i(\theta_{n;k} + \theta_{m;-k}) \right], \quad (2.19)$$

$$\theta_{n;k} = -\theta_{n;-k}, \quad (2.20)$$

where the $\theta_{n;k}$ are real phases. Again we see that (2.8) is satisfied. Let us give the $\theta_{n;k}$ values chosen at random in the interval $(0, 2\pi)$. The choice is to be made independently for each pair of indices n, k , subject only to (2.20). We shall call the result the ring model, for reasons which will become clear shortly. It represents a rather more drastic mutilation of the true Hamiltonian than does the ladder model. Because the phases $\theta_{n;k}$ fluctuate randomly as k changes, the present $V^{n,m}(x)$ are strange potentials which spread out irregularly over the entire cyclic cube.

The ring model Hamiltonian also has a boundedness property in common with the true Hamiltonian, but a different one than we noted for the ladder model. Let us formally define a self-interaction potential by extending (2.6), (2.7), and (2.19), without change, to the case $n = m$. Then we may rewrite the model interaction Hamiltonian in the form

$$H_1 = \frac{1}{2} \sum_{n,m} V^{n,m}(x_n - x_m) - \frac{1}{2} NV(0), \quad (2.21)$$

where the summation now admits $n = m$. Using (2.6), (2.19), and (2.20), we find

$$H_1 = \frac{1}{2} \sum_k V_k \rho_k \rho_k^* - \frac{1}{2} NV(0), \quad (2.23)$$

where

$$\rho_k = \sum_n \exp[i(k \cdot x_n + \theta_{n;k})]. \quad (2.24)$$

Now suppose that V_k is non-negative for all k . Then $\sum_k V_k \rho_k \rho_k^*$ is a non-negative operator, and it follows that the expectation of the potential energy per particle in any quantum-mechanical state is bounded from below by $-\frac{1}{2} V(0)$.

In the true problem all the $\theta_{n;k}$ are zero, and ρ_k is a density-operator Fourier component, as introduced by Pines and Bohm¹⁶ and others. In the ring model, we may call ρ_k an effective density component.

The conditions $V(x) \geq 0$ (all x) and $V_k \geq 0$ (all k) are not mutually exclusive, but they do not imply each other. The bounds we have derived therefore suggest that the ladder and ring models have inequivalent domains of validity. Consider, for example, the modified coulomb potential

$$V_k = \Omega^{-1} 4\pi e^2 \exp(-a|k|) k^{-2} \quad (|k| \geq 1/\ell),$$

$$V_k = 0 \quad (|k| < 1/\ell), \quad (2.24)$$

where a and ℓ provide, respectively, a short-range and long-range cut-off. V_k is non-negative and $V(0)$ is finite. Thus the ring model Hamiltonian

has a finite lower bound per particle and may be expected to yield healthy results. On the other hand, $V(x) \geq 0$ is not satisfied for large x , and we cannot make a similar prediction for the ladder model.

If we let $\epsilon \rightarrow \infty$, then $V(0)$ approaches a finite limit, and we conclude that the long-range character of the coulomb potential should not pose difficulties for the ring model. In the limit $a \rightarrow 0$, however, we have $-\frac{1}{2} V(0) \rightarrow -\infty$. In the true problem, the V_k for very high k give a purely repulsive contribution to $V(x)$ and cannot actually cause H_1 to be unbounded from below. In the ring model, however, the very high k give rise to attractive as well as repulsive regions in the $V^{n,m}(x)$, because of the fluctuating phases of the $V_k^{n,m}$. Thus we may anticipate trouble in the limit $a \rightarrow 0$. We shall see shortly that it actually occurs, at least in the classical case.

The B_α may be evaluated for the ring model by expanding the $f^{n,m}(x)$ as power series in $-\beta$, expanding the $V^{n,m}(x)$ in Fourier series, and then performing the space integrations. We thereby find

$$B_1 = \Omega N^{-2} \sum_{n,m} \left[-V_0^{n,m} + \frac{1}{2}(-\beta)^2 \sum_k V_k^{n,m} V_{-k}^{n,m} + \frac{1}{3!} (-\beta)^3 \sum_{k,k'} V_k^{n,m} V_{k'}^{n,m} V_{-k-k'}^{n,m} + \dots \right]. \quad (2.25)$$

By (2.19) and (2.20), we find

$$V_0^{n,m} = V_0, \quad V_k^{n,m} V_{-k}^{n,m} = V_k V_{-k}.$$

Thus the first two terms on the right side of (2.25) are unaffected by the averaging over n and m . All the higher terms, however, involve phases which fluctuate randomly as n and m are varied, except when all the summed indices k, k', \dots are either equal and opposite in pairs or zero. The consequence is that none of the higher terms makes a contribution to B_1 in the limit $N \rightarrow \infty, \Omega \rightarrow \infty$.

We shall illustrate by considering the term containing $(-\beta)^3$.

The random phase of the summand is

$$(\theta_{n;k} + \theta_{m;k'}) + (\theta_{n;k'} + \theta_{m;-k'}) + (\theta_{n;-k-k'} + \theta_{m;k+k'}).$$

By (2.20), this expression vanishes for $k = 0, k' = 0$, or $k + k' = 0$.

However, it follows readily from the restrictions on $V(x)$, stated after (2.3), that the total contribution to B_1 from these restricted wave-vector combinations vanishes in the limit. For the remaining wave-vector combinations, the phase of the summand changes at random with change of n and m . For a given k and k' , the averaging over n and m therefore reduces the contribution to B_1 by a factor $\sim N^{-1} = 1/\sqrt{(N^2)}$ from its value in the true problem. The consequence is that the total contribution of the $(-\beta)^3$ term vanishes in the limit. Similar arguments show that all the higher terms vanish also. Thus we have

$$B_1 = \Omega \left[-\beta V_0 + \frac{1}{2} \beta^2 \sum_k (V_k)^2 \right], \quad (2.26)$$

where we note $V_k = V_{-k}$. In obtaining (2.26), we use the fact that the expansion of $f^{n,m}(x)$ in powers of $-\beta$ is absolutely convergent for all β , if $V(x)$ obeys the restrictions imposed after (2.3).

The higher B_α may be evaluated by similar analysis. The result is that the only irreducible Mayer diagrams which give nonvanishing contributions in the limit are the ring diagrams, the first three of which are shown in Figs. 1b and 1c. The surviving contributions from the ring diagrams give

$$B_\alpha = \frac{1}{2} \sum_k (-\beta)^{\alpha+1} n^\alpha (V_k)^{\alpha+1} \quad (\alpha \geq 2). \quad (2.27)$$

The surviving contributions arise as the products of the terms $\propto -\beta$ in the expansions of all the f factors occurring in the ring diagram integrands. To see how they survive, consider Fig. 1b. The surviving contribution from this diagram is

$$\frac{1}{2} N^{-3} \sum_{n,m,\ell} \sum_k (-\beta)^3 n^2 V_k^{n,m} V_k^{m,2} V_k^{\ell,n},$$

and the phase of the summand is

$$(\theta_{n;k} + \theta_{m;-k}) + (\theta_{m;k} + \theta_{\ell;-k}) + (\theta_{\ell;k} + \theta_{n;-k}),$$

which vanishes by (2.20).

Inserting (2.26) and (2.27) in (2.11), and performing the sum over α ,¹⁷ we find

$$A - A_C = \frac{1}{2} \rho n V_0 - \frac{1}{2} (\beta \rho)^{-1} n^{-1} \sum_k \left[\beta \rho V_k - \ln(1 + \beta \rho V_k) \right]. \quad (2.28)$$

It is of interest to compare (2.28) with the well-known result

$$A-A_0 = -\frac{1}{2} \rho \beta^{-1} \Omega f_0 - \frac{1}{2} (\beta \rho)^{-1} \Omega^{-1} \sum_k \left[-\rho \Omega f_k - \ln(1 - \rho \Omega f_k) \right. \\ \left. - \frac{1}{2} \rho^2 \Omega^2 f_k^2 \right], \quad (2.29)$$

where f_k is defined by

$$f(x) = \sum_k f_k \exp(ik \cdot x),$$

which Montroll and Mayer¹⁷ obtained by summing all the ring diagrams for the true problem. We shall find that (2.28), and not (2.29), represents the classical limit of the quantum-mechanical ring summation to be carried out in Sec. 4.¹⁸

From (2.28), we see that $A-A_0$ is bounded from below ($V_k \geq 0$) by

$$-\frac{1}{2} \sum_k V_k = -\frac{1}{2} V(0),$$

which agrees with the rigorous bound we have previously found for the ring-model potential energy. As in the case of the ladder model, this provides some reassurance as to the validity of our formal procedure. It is clear that if $V_0 = 0$, then $A-A_0$ will actually approach the absolute lower bound as $\beta \rightarrow \infty$. [The \ln term in (2.28) gives a vanishing contribution in this limit.]

If V_k is given by (2.24), we find that $A-A_0$ converges in the limit $\ell \rightarrow \infty$ and/or $\beta \rightarrow \infty$. This supports our anticipation that the long-range

part of the potential should not pose difficulties for the ring model. It should be noted that the derivation of (2.28) with potential (2.24) requires that l be kept finite until after the limit $q \rightarrow \infty$ is taken. Otherwise, the assumption $V_k = O(k^{-1})$ is violated for very low k .

If now we take $a = 0$, we find $A - A_0 \rightarrow -\infty$ as $\beta \rightarrow \infty$. Thus, as we anticipated might be so, the ring model is not an admissible approximation in this case. The situation may be substantially improved in the quantum theory, however.

2.4 Random-Coupling and Hartree-Fock Models

We wish now to examine two simpler distinguishable-particle models. In common with the ladder and ring models, they are of interest because their classical thermodynamics represents limits for corresponding fermion and boson models.

Let us now specialize $\phi_{n,m;k}$ to the form

$$\phi_{n,m;k} = \exp(i\theta_{n,m;k}), \quad (2.30)$$

with

$$\theta_{n,m;k} = -\theta_{m,n;k}, \quad \theta_{n,m;k} = -\theta_{n,m;-k}, \quad (2.31)$$

where the $\theta_{n,m;k}$ are real phases. Again (2.8) is satisfied. Let $\theta_{n,m;k}$ give the $\theta_{n,m;k}$ values in the interval $(0, \pi)$ determined by independent, random choices for all the combinations of indices, subject only to (2.31). We shall call this the random-coupling model.

There appears to be no lower bound to the potential energy per particle in the random coupling model if we take the limit $N \rightarrow \infty$. Consequently, we cannot be sure that the model has any thermodynamic validity. We shall return to this question in a moment.

The B_α for the random-coupling model may be determined by the same formal procedure as we used for the ring model. The result is that B_1 has the value (2.26) and that all the higher B_α vanish in the limit $N \rightarrow \infty$, $\Omega \rightarrow \infty$. The results for A and p are

$$A - A_0 = \frac{1}{2} \rho \Omega V_0 - \frac{1}{4} \rho \beta \Omega \sum_k V_k^2 \quad (2.32)$$

and

$$p = \beta^{-1} \rho + \frac{1}{2} \rho^2 \Omega V_0 - \frac{1}{4} \beta \rho^2 \Omega \sum_k V_k^2. \quad (2.33)$$

If (2.17) is expanded in powers of $-\beta$, and then expressed in terms of Fourier coefficients, it is easy to verify that (2.32) represents that part of (2.17) which is also contained in (2.28). That is to say, the only contributions to A which survive in the random-coupling model are those which survive in both the ladder and ring models.

From (2.33) we see that if ρ and β are high enough we have $(\partial p / \partial \rho)_\beta < 0$, regardless of the form of $V(x)$. The instability to collapse thereby indicated,¹⁵ is associated with the lack of a lower bound to the model potential energy. However, if ρ and β are low enough, (2.33) suggests that the random-coupling model may have a stable thermodynamics. We choose to regard that indication with caution.

Our final model is the Hartree-Fock model, which we construct by taking

$$V_0^{n,m} = V_0, \quad V_k^{n,m} = 0 \quad (k \neq 0). \quad (2.34)$$

This is a zeroth model in the sense that there are no randomly chosen parameters at all. It corresponds simply to having each particle move in the uniform potential obtained by averaging the true fields of the other particles over all possible configurations. Only k_1 is nonvanishing in the limit $\Omega \rightarrow \infty$, and we have

$$A - A_0 = \frac{1}{2} \rho \Omega V_0. \quad (2.35)$$

3. MODELS FOR FERMIONS AND BOSONS

3.1. Nature of the Models

The models described in Sec. 2 involve interaction potentials which are different for different pairs of particles. They are therefore meaningless for indistinguishable particles. In order to construct stochastic models for fermion and boson systems, let us replace (2.1) by the second-quantized true Hamiltonian

$$H = H_0 + H_1, \quad H_0 = \sum_k \epsilon_k a_k^\dagger a_k, \quad (2.1)$$

$$H_1 = \frac{1}{2} \sum_{kpr} V_{k-c, k+p, r+c} a_k^\dagger a_r^\dagger a_r a_c. \quad (2.2)$$

Here a_k^\dagger and a_k are fermion or boson creation and destruction operators for momentum k , ϵ_k is the free-particle energy $\frac{1}{2} k^2$, and we take $n = 1$.

The commutation relations are

$$[q_k, q_p]_{\pm} = 0, \quad [q_k, q_p^{\dagger}]_{\pm} = \delta_{kp}, \quad (3.3)$$

where the plus sign is for fermions and the minus for bosons.

As the general model interaction Hamiltonian, we take

$$H_1 = \frac{1}{2} \sum_{kprs} V_{k-s} \phi_{kprs} \delta_{k+p, r+s} q_k^{\dagger} q_p^{\dagger} q_r q_s, \quad (3.4)$$

where the ϕ_{kprs} are c-number parameters which play a role analogous to that of the $\phi_{n,m;k}$. We leave H_0 unaltered. In correspondence to (2.8), we impose the conditions

$$\phi_{kprs} = \phi_{srpk}^*, \quad \phi_{kprs} = \phi_{pkrs}. \quad (3.5)$$

The first of these relations insures the Hermiticity of H_1 . The second is suggested by the invariance of (3.2) to the 'particle exchange' $(k,s) \rightleftharpoons (p,r)$.

We shall obtain the fermion and boson versions of the ladder, ring, random-coupling, and Hartree-Fock models by making specialized stochastic assignments of values to the ϕ_{kprs} . The ϕ_{kprs} will all have unit modulus in the models we shall examine here, except in the Hartree-Fock model, where most of the ϕ_{kprs} will vanish. In Secs. 4 and 5 we shall develop an appropriate propagator formalism for the fermion and boson models and find closed equations which determine the propagators for each model. We shall put off until Sec. 6 a demonstration of the relations among the fermion, boson, and distinguishable-particle models.

3.2. Ladder Model

To construct the fermion or boson ladder model, we take

$$\phi_{kp rs} = \exp[i(-\theta_{pk} + \theta_{rs})], \quad (3.6)$$

with

$$\theta_{kp} = \theta_{pk}. \quad (3.7)$$

We then determine the real phase θ_{kp} for each pair k, p by a random choice in the interval $(0, 2\pi)$. The choices are all independent, subject only to (3.7).

Let us define the quantities

$$\begin{aligned} X(x', x) &= \Omega^{-1} \sum_{rs} q_r q_s \exp[i(r \cdot x' + s \cdot x + \theta_{rs})], \\ X^\dagger(x', x) &= \Omega^{-1} \sum_{rs} q_r^\dagger q_s^\dagger \exp[-i(r \cdot x' + s \cdot x + \theta_{rs})]. \end{aligned} \quad (3.8)$$

In the true problem (all $\theta_{rs} = 0$), $X(x', x)$ is simply the two-particle amplitude $\psi(x')\psi(x)$, where $\psi(x)$ is the destruction field in x space. We may call $X(x', x)$ the effective two-particle amplitude in the ladder model. By straightforward Fourier analysis, we find

$$H_1 = \frac{1}{2} \iint V(x-x') X^\dagger(x', x) X(x', x) dx' dx. \quad (3.9)$$

If $V(x) \geq 0$ for all x , H_1 is a positive-definite operator, and it follows that the eigenvalues of H_1 are all non-negative. This is the same result which we obtained in Sec. 2 for the distinguishable-particle ladder model.

It is not obvious that the present model will be an admissible approximation to the true problem if $V(x)$ is a hard-sphere potential, although this was clearly the case for the distinguishable-particle ladder model. A sufficient condition for admissibility would appear to be that the relation

$$\chi(x', x) |\bar{\Phi}\rangle = 0, \quad (|x-x'| \leq r_0), \quad (3.10)$$

where r_0 is the hard-sphere diameter, be satisfied for as rich a manifold of states $\bar{\Phi}$ in the model as in the true problem. We have not investigated this question.

3.3. Ring Model

To construct the fermion or boson ring model, we take

$$\phi_{kprs} = \exp \left[i(\bar{\theta}_{ks} + \bar{\theta}_{pr}) \right], \quad (3.11)$$

where

$$\bar{\theta}_{ks} = -\bar{\theta}_{sk}. \quad (3.12)$$

We fix the real phases $\bar{\theta}_{ks}$ by random choices in the interval $(0, 2\pi)$, subject only to (3.12).

In analogy to (2.23), let us introduce the effective density-component operators

$$\rho_m = \sum_k q_k^\dagger q_{k+m} \exp(i\bar{\theta}_{k, k+m}). \quad (3.13)$$

By (3.12), they satisfy $\rho_m = \rho_{-m}^\dagger$. It follows from (3.3) and (3.12) that

for either fermions or bosons the ring model H_1 may be rewritten

$$H_1 = \frac{1}{2} \sum_k V_k \rho_k^\dagger \rho_k + \frac{1}{2} V(0)N, \quad (3.14)$$

where

$$N = \sum_k N_k, \quad N_k = q_k^\dagger q_k.$$

As in (2.22), we note that the first term on the right side of (3.14) is a positive-definite operator if $V_k \geq 0$ for all k . It follows that the fermion and boson ring models exhibit the same lower bound on H as did the distinguishable-particle ring model.

A third model, which has no analog in the distinguishable case, may be constructed by taking

$$\phi_{kprs} = \exp[i(\bar{\theta}_{kr} + \bar{\theta}_{ps})] \quad (3.15)$$

and requiring the $\bar{\theta}_{kr}$ to obey (3.12). We may call this the exchange model. Hybrid models may also be constructed, by taking ϕ_{kprs} as a linear combination of the forms for the ladder, ring, and exchange models. We shall not discuss these cases in this paper.

3.4. Random-Coupling and Hartree-Fock Models

To construct the fermion and boson versions of the random-coupling model, we take

$$\phi_{kprs} = \exp(i\theta_{kprs}), \quad (3.16)$$

with

$$\theta_{kprs} = -\theta_{srpk}, \quad \theta_{kprs} = \theta_{pkrs}, \quad \theta_{kprs} = \theta_{pkrs}, \quad (3.17)$$

and fix the phases θ_{kprs} by independent random choices for each combination of indices (k,p,r,s) , subject only to (3.17). As in the distinguishable-particle random coupling model, there appears to be no lower bound on the potential energy per particle when the system is infinite. This suggests that results obtained from the random-coupling model be viewed with skepticism. It perhaps should be pointed out that our random-coupling models are unrelated to the random-phase approximation employed by Pines and Bohm¹⁶ and others. We make no assumption about the phase correlations among the dynamic variables.

The fermion or boson Hartree-Fock model is given by the assignment

$$\phi_{kppk} = \phi_{kpkp} = 1, \quad \phi_{kprs} = 0 \quad (k \neq r \text{ or } s). \quad (3.18)$$

This model contains no randomly chosen parameters. We shall see in Sec. 5 that it yields simply the Hartree-Fock approximation to the true problem, in the limit $\Omega \rightarrow \infty$.

4. TEMPERATURE-DOMAIN PROPAGATOR FORMALISM

The equilibrium statistical mechanics of the fermion and boson models can be investigated most neatly by means of the temperature-domain propagator formalism and its associated diagram technique.^{2,5,6,8} Since our models differ from the true Hamiltonian only by the replacement

$$V_{k-s} \delta_{k+p, r+s} \rightarrow V_{k-s} \phi_{kprs} \delta_{k+p, r+s}, \quad (4.1)$$

the existing techniques may be taken over with only minor and obvious changes. We shall summarize the resulting formalism in the present section.¹⁹

Let us define the temperature-domain propagator $S_k(u, u')$ by

$$S_k(u, u') = - \left\langle T[q_k(u) q_k^\dagger(u')] \right\rangle \quad (u, u' \text{ real}), \quad (4.2)$$

where

$$q_k(u) = e^{uH} q_k e^{-uH}, \quad q_k^\dagger(u) = e^{uH} q_k^\dagger e^{-uH}. \quad (4.3)$$

The ordering operator T is defined by

$$\begin{aligned} T[q_k(u) q_k^\dagger(u')] &= q_k(u) q_k^\dagger(u') & (u > u'), \\ T[q_k(u) q_k^\dagger(u')] &= \mp q_k^\dagger(u') q_k(u) & (u \leq u'). \end{aligned} \quad (4.4)$$

In (4.4) and in all subsequent expressions where a plus-minus or minus-plus sign occurs, the upper sign refers to fermions and the lower to bosons. The brackets $\langle \rangle$ denote an average over the grand canonical ensemble. For any operator B ,

$$\langle B \rangle \equiv \text{Tr} \left\{ e^{-\beta(H - \mu N)} B \right\} / \text{Tr} \left\{ e^{-\beta(H - \mu N)} \right\}, \quad (4.5)$$

where N is defined below (3.14) and μ is the chemical potential.

The propagator has a Fourier expansion of the form

$$S_k(u, u') = \beta^{-1} \sum_{a=-\infty}^{\infty} S_k(\zeta_a) \exp \left[\zeta_a (u' - u + \delta) \right], \quad (4.6)$$

where

$$\begin{aligned}\zeta_a &= \mu + i\pi(2a+1)\beta^{-1} && (\text{fermions}), \\ \zeta_a &= \mu + 2i\pi a\beta^{-1} && (\text{bosons}),\end{aligned}\tag{4.7}$$

and a takes all integer values. The quantity δ is an infinitesimal real, positive number. We shall call $S_k(\zeta_a)$ a propagator also, and we shall call ζ_a an 'energy'.

The complete thermodynamic behavior of the system can be obtained from $S_k(\zeta_a)$. The mean number of particles at a given temperature and chemical potential is

$$N(\beta, \mu) = \sum_k \bar{N}_k, \quad \bar{N}_k = \pm \beta^{-1} \sum_a S_k(\zeta_a) \exp(\zeta_a \delta), \tag{4.8}$$

where the $\bar{N}_k \equiv \langle N_k \rangle$ are the mean occupation numbers. The mean energy also has a direct expression. Using (3.1), (3.3), (3.4), and (4.3), we find

$$\pm \sum_k \left[\partial S_k(u, u') / \partial u' \right]_{u'=u} = \langle H_0 \rangle + 2 \langle H_1 \rangle, \tag{4.9}$$

and we note that $\langle H_0 \rangle = \pm \sum_k \epsilon_k S_k(u, u)$. Then it follows from (4.6) that the mean energy $E(\beta, \mu)$ is given by²⁰

$$E(\beta, \mu) = \pm \frac{1}{2} \beta^{-1} \sum_{k,a} (\epsilon_k + \zeta_a) S_k(\zeta_a) \exp(\zeta_a \delta). \tag{4.10}$$

The entropy, pressure, and other thermodynamic quantities can be found from $N(\beta, \mu)$ and $E(\beta, \mu)$. [Alternatively, the thermodynamic potential may be obtained from $S_k(\zeta_a)$ by an integration over an interaction strength parameter.^{8]}

The propagator for free particles is

$$S_k^{(0)}(\xi_k) = (\xi_k - \epsilon_k)^{-1}. \quad (4.11)$$

The coupled-particle propagator $S_k(\xi_k)$ may be expressed in terms of $S_k^{(0)}(\xi_k)$ by a linked-diagram expansion constructed according to the following rules:

1. Call the diagram part shown in Fig. 8a a vertex. A vertex consists of two solid-line junctions connected by a dashed line. 'Line' hereafter will mean solid line except where noted.
2. For each positive integer n , take n vertices and join incoming with outgoing lines in pairs so as to form, just once, all possible distinct, linked diagrams with just one incoming and one outgoing external line. Linked diagrams are those which do not consist of disconnected parts. External lines are those which leave or enter the diagram. In reckoning distinctness, the n original vertices are considered indistinguishable and the two solid-line junctions in any vertex are considered indistinguishable. However, incoming lines are distinct from outgoing lines. Examples: Figs. 6a and 8a are distinct. But Figs. 6a and 7a are not.
3. Label the external lines with momentum k . Label the internal lines with momenta k', k'', \dots . In addition, associate the 'energy' ξ_k with the external lines, and 'energies' $\xi_{k'}, \xi_{k''}, \dots$ with the internal lines.

4. With each line, external or internal, associate a factor $\xi_p^{(0)}(\xi_b)$, where p is the momentum labeling the line and ξ_b is the associated 'energy'. Special case: Include an additional factor $\exp(\xi_b \delta)$ if the beginning and termination of the line are in the same vertex.
5. With each vertex, at which are joined lines with momentum labels p, q, r, s and respective 'energies' $\xi_b, \xi_c, \xi_d, \xi_e$ as shown in Fig. 2b, associate a factor

$$-\beta^{-1} \phi_{pqrs} v_{p-s} \delta_{p+q, r+s} \delta_{b+c, d+e}$$

Note: This rule is ambiguous with respect to the exchange $(p, s) \rightleftharpoons (q, r)$. By (2.3) and (3.5), however, the factor called for by the rule is invariant in value under the exchange.

6. For fermions only: Associate with each diagram a factor $(-1)^l$, where l is the number of closed solid-line loops in the diagram.
7. To form the contribution of a given diagram, multiply together all the factors introduced by rules 4, 5, and 6 and then sum over all the momenta k', k'', \dots and 'energies' ξ_a, ξ_a'', \dots associated with the internal lines.
8. To form $S_k(\xi_a)$, first sum the contributions given by rule 7 for all the diagrams admitted by rule 2. Then add the contribution $S_k^{(0)}(\xi_a)$, which is associated with the zeroth order ($n = 0$) diagram Fig. 3a.

We shall call the expansion for $S_k(\xi_a)$ generated by rules 1 - 8 the primitive linked-diagram expansion. A more compact expansion, which

we shall call the irreducible linked-diagram expansion, may be constructed by replacing rules 2 and 4 with the following altered rules:

2'. Retain only those diagrams admitted by rule 2 which do not contain self-energy parts. We shall call these irreducible diagrams. (A self-energy part is a part of a diagram which contains at least one but not all the vertices and which is connected to the rest of the diagram by just one outgoing and one incoming line.)

4'. In rule 4, replace each factor $S_p^{(0)}(\zeta_b)$ by a factor $S_p(\zeta_b)$.
Exception: With the outgoing external line associate the factor $S_k^{(0)}(\zeta_a)$ as before.

The primitive diagram expansion gives $S_k(\zeta_a)$ as an infinite sum of integrals (we consider the case $\Omega \rightarrow \infty$) over the known quantities $S_k^{(0)}(\zeta_a)$. In contrast, the irreducible expansion is really an infinite-series integral equation for $S_k(\zeta_a)$. A convenient way to express the irreducible expansion is as follows: We define $M_k(\zeta_a)$ by

$$S_k(\zeta_a) = \left[\zeta_a - \epsilon_k - M_k(\zeta_a) \right]^{-1}. \quad (4.12)$$

Then the irreducible linked-diagram expansion for $M_k(\zeta_a)$ is the same as that for $S_k(\zeta_a)$, except for the changes expressed by the following further rule alteration:

4". In rule 4', omit entirely the factors for the two external lines.

8'. In rule 8, omit the contribution of the zeroth-order diagram.

The use of the rules will be illustrated by the examples treated in Sec. 5. If we take $\phi_{kprs} = 1$ for all k, p, r, s , then the rules we have given yield the established propagator expansions for the true problem.

5. PROPAGATOR EQUATIONS FOR THE MODELS

5.1. Underlying Assumptions

We shall now show that our fermion and boson models lead to closed integral equations for $S_k(\xi_a)$ in the limit $\Omega \rightarrow \infty$ with fixed μ or ρ . We wish first to state clearly the assumptions which underlie the analysis:

1. As in Sec. 2, we restrict $V(x)$ to be a smooth, bounded function such that $|V_k| \leq O(k^{-2})$, $k \rightarrow \infty$.

2. We assume that all the sums over intermediate momenta which occur in any given order of the primitive linked-diagram expansion converge at infinity. More precisely, we assume that, for given k and a , the contributions to $S_k(\xi_a)$ which involve intermediate momenta higher than some given momentum k_{\max} vanish as $k_{\max} \rightarrow \infty$. Moreover, we assume that they vanish in a manner independent of Ω as $\Omega \rightarrow \infty$. We believe that this assumption actually follows from assumption 1, but we shall not try to prove this here.

3. As in Sec. 2, we assume that $V_k = O(\Omega^{-1})$ for all k as $\Omega \rightarrow \infty$. This means that for long-range potentials a cut-off length ℓ must be employed as in (2.24). We take the limit $\ell \rightarrow \infty$ only after the limit $\Omega \rightarrow \infty$ has been performed.

4. For every k and α we assume that $S_k^{(0)}(\xi_\alpha)$ approaches a limit independent of Ω as $\Omega \rightarrow \infty$ with Ω constant. This excludes from our present considerations boson systems below the Einstein-Bose condensation temperature.

5. The final assumption involves a deep-lying convergence question corresponding to that which arose in Sec. 2. We shall assume, for each of the models, that large classes of diagrams give a vanishing contribution to $S_k(\xi_\alpha)$ in the limit $\Omega \rightarrow \infty$, up to any given order of diagram. On this basis, we shall assume that these classes do not contribute when summed to all orders. It will not follow from our analysis that this is actually so. The reason is that the diagrams of order N ($=\rho\Omega$) and higher are enormous in number for large Ω , and it will not be clear that cancellations due to the randomness of the ϕ_{kpr} will suppress the contribution of these diagrams as they do contributions of finite order.

The necessity for assumptions 3 and 4 will be eliminated by the generalized treatment given in the following paper. There we construct models for systems of any size and obtain closed propagator equations without taking the limit $\Omega \rightarrow \infty$. The final equations are identical with those to be derived here, and they justify the latter in cases where assumptions 3 and 4 are not satisfied. In particular, they establish the closed model equations for condensed boson systems. The generalized treatment provides much neater derivations of all the results to be obtained in Sec. 5. We do not employ it at the outset because it requires an unfamiliar and more elaborate formalism.

Assumption 5 also is best examined by the methods of the following paper. The approach to this question adopted there is to consider the propagators in the real-time domain, rather than the temperature domain, and to regard them as the limits of more general quantities (correlation and Green's functions) which are defined for non-equilibrium as well as equilibrium. Linked diagram expansions exist which give the evolution of the correlation and Green's functions forward in time from a given initial statistical state. As in the present case, these expansions can be formally summed and expressed by closed equations for each of our models.

A new feature, however, is that the evolution in time can also be examined by an alternate method which seems genuinely independent of perturbation expansions. One can replace the exact differential equations of evolution by corresponding difference equations involving small time increments. In contrast to a perturbation expansion (which is akin to a Taylor series) such a procedure should converge, as the increment size is decreased to zero, whenever the differential equations themselves are meaningful. This permits an examination of assumption 5 from a new point of view. Although the analysis we shall present in the following paper is not rigorous, we feel that it provides substantial support for the validity of our closed model equations.

5.2. Hartree-Fock and Random-Coupling Models

The derivation of closed propagator equations is simplest for the Hartree-Fock model. Consider the primitive linked-diagram expansion for $S_k(\zeta_a)$. There are two distinct first-order diagrams, and they are shown

in Figs. 3b and 3c. By the rules of Sec. 4, the contributions of these diagrams involve the factors ϕ_{kppk} and ϕ_{kpkp} , respectively, but no other ϕ factors. Therefore, by (3.18), their contributions are identical in the Hartree-Fock model and in the true problem.

However, consider Fig. 4a. The contribution of this second-order diagram to the primitive expansion for $S_k(\xi_a)$ is

$$\begin{aligned} & + \beta^{-2} \sum_{ps} \phi_{kp rs} \phi_{sr pk} V_{k-s} V_{s-k} \sum_{bc} S_k^{(0)}(\xi_a) S_p^{(0)}(\xi_b) \\ & \times S_s^{(0)}(\xi_c) S_r^{(0)}(\xi_d) S_k^{(0)}(\xi_a), \end{aligned} \quad (5.1)$$

where $r = k + p - s$, $d = a + b - c$, by momentum and 'energy' conservation. By (3.18), the only surviving terms in the sum are those for which either $s = k$, $r = p$ or $r = k$, $s = p$. Thus, there is only one free intermediate momentum, which we may take as p . Now as $\Omega \rightarrow \infty$, the number of allowed momenta p in any given volume of momentum space is $\propto \Omega$. It then follows from assumptions 2, 3, and 4 of Sec. 5.1 that the contribution (5.1) vanishes as Ω^{-1} .

If similar considerations are applied to the rest of the primitive linked diagrams, it is possible to verify the following result: The only diagrams which survive in the limit $\Omega \rightarrow \infty$ are those for which momentum conservation alone assures that the ϕ product given by the rules of Sec. 4 consists wholly of factors of the form ϕ_{ppqq} or ϕ_{ppqp} . Such diagrams give the same contribution as they do in the true problem. For every other diagram of finite order, (3.18) so restricts the summations over intermediate momenta that the result vanishes as some positive integral power of Ω^{-1} .

It is ~~easy~~ to see from the rules of Sec. 4 that the higher surviving primitive diagrams, which we have just specified, are simply those which can be obtained from Figs. 3b and 3c by repeatedly inserting these first-order diagrams into themselves and into each other as self-energy parts. (See Fig. 5.) Now let us invoke assumption 5 of Sec. 5.1. It then follows that Figs. 3b and 3c are the only diagrams which survive in the irreducible expansion for $S_k(\xi_a)$ in the limit $\Omega \rightarrow \infty$. We may see this by noting that the primitive expansion can be recovered from the irreducible expansion by taking every factor S which occurs in the latter and replacing it by its own primitive expansion. If diagrams other than Figs. 3b and 3c occurred in the irreducible expansion, then it is clear that the primitive expansion for $S_k(\xi_a)$ thus recovered would contain diagrams other than those we have specified.

Using the rules of Sec. 4 to evaluate the contribution to $M_k(\xi_a)$ of the two surviving irreducible diagrams, we find

$$M_k(\xi_a) = \beta^{-1} \sum_{pb} (\pm V_0 - V_{k-p}) S_p(\xi_b) \exp(\xi_b \delta), \quad (5.2)$$

where we have noted (2.3). The first term on the right side of (5.2) arises from Fig. 3b and the second from Fig. 3c. Upon inserting (5.2) into (4.12), we obtain a closed integral equation for $S_k(\xi_a)$ for the Hartree-Fock model. Equation (5.2) may be rewritten in the form

$$M_k(\xi_a) = \sum_p (V_0 \mp V_{k-p}) \bar{N}_p, \quad (5.3)$$

where we use (4.8). The parts of this result involving V_0 and V_{k-p} are,

respectively, the direct and exchange parts of the effective potential which is obtained in the usual Hartree-Fock approximation to the true problem.

Let us consider next the random-coupling model. By (3.16) and (3.17), we find

$$\phi_{kppk} = 1, \quad \phi_{kpkp} = 1, \quad \phi_{kprs}\phi_{srpk} = 1, \quad \phi_{kprs}\phi_{srkp} = 1. \quad (5.4)$$

It then follows from the rules of Sec. 4 that Figs. 3b, 3c, 4a and 4b all survive in the primitive expansion for $S_k(\xi_a)$ and give the same contributions as in the true problem.

However, consider Fig. 6a. The contribution which it makes to the primitive expansion for $S_k(\xi_a)$ is of the form

$$\begin{aligned} & \pm \beta^{-3} \sum_{prsr's'} \phi_{kprs}\phi_{srr's'}\phi_{s'r'pk} \delta_{k+p, r+s} \delta_{r+s, r'+s'} \delta_{r'+s', p+k} \\ & \times V_{k-s} V_{s-s'} V_{s'-k} \sum_{(\text{energies})} (\text{product of } S^{(0)} \text{ factors}). \quad (5.5) \end{aligned}$$

There is an identity among the conservation conditions given by the three Kronecker symbols. Consequently there are three independent intermediate momenta, which we may take as p , s , and s' . For special values of these momenta, the ϕ product is unity by (5.4). However, in correspondence to the result noted above for the Hartree-Fock model, it is easy to see that these special values give a vanishing contribution to $S_k(\xi_a)$ when $\Omega \rightarrow \infty$. Except for these restricted momentum values,

the ϕ product will have a phase which, by (3.16) et seq., fluctuates at random with change of p , s , and s' .

Now let us divide the momentum space into small regions, of 'volume' Δ , such that $S_p^{(0)}(\xi_b)$ exhibits negligible change if p varies within a given region. By assumption 4 of Sec. 5.1, this should be possible in the limit $\Omega \rightarrow \infty$. Now as $\Omega \rightarrow \infty$, the density of allowed modes in momentum space is $\sim \Omega$. Hence, in the summation over momenta in (5.5), the number of terms for p , s , and s' within given small regions will be $\sim (\Omega\Delta)^3$. Let us consider the contribution from those terms in which the phase of the ϕ product fluctuates at random with change of p , s , and s' . As we have just noted, these constitute all but a negligible fraction of the terms. Because of the phase-fluctuation, the total contribution of these terms will be down by a factor $\sim (\Omega\Delta)^{-3/2}$ from the value it would have in the true problem. Since this factor vanishes as $\Omega \rightarrow \infty$, it follows from assumptions 2 and 3 of Sec. 5.1 that the contribution to $S_k(\xi_a)$ from Fig. 6a vanishes in the limit. Our argument, of course, assumes a typical assignment of values to the randomly chosen parameters θ_{kprs} (cf. the discussion in Sec. 2.2).

Similar analysis may be applied to the higher diagrams in the primitive expansion for $S_k(\xi_a)$. The result is that the only diagrams which survive are those for which momentum conservation alone assures that the ϕ product consists entirely of factors and/or factor-pairs of the forms shown in (5.4). Any other diagram gives a contribution which vanishes as some negative power of Ω as $\Omega \rightarrow \infty$. The surviving diagrams can be seen to be those which can be constructed from Figs. 3b, 3c, 4a,

and 4b by inserting these same four diagrams repeatedly as self-energy parts, in correspondence to the situation for the Hartree-Fock model. It follows from this that the only surviving diagrams in the irreducible expansion for $S_k(\zeta_a)$ are Figs. 3b, 3c, 4a, and 4b. Again, assumption 5 of Sec. 5.1 is implicit in the argument.

Combining the contributions of the four surviving irreducible diagrams according to the rules of Sec. 4, we find

$$M_k(\zeta_a) = \sum_p (V_0 + V_{k-p}) \bar{N}_p$$

$$+ \beta^{-2} \sum_{psbc} V_{k-s} (V_{k-s} + V_{p-s}) S_p(\zeta_b) S_s(\zeta_c) S_{k+p-s}(\zeta_{a+b-c}), \quad (5.6)$$

where, again, we note (4.8).

If the third of constraints (3.17) were relaxed in assigning random values to the Θ_{kprs} , we would obtain a version of the random-coupling model in which the exchange diagram Fig. 4b did not survive. The corresponding expression for $M_k(\zeta_a)$ would not include the term in (5.6) which involves V_{p-s} .

5.3. Ring and Ladder Models

The results described above for the Hartree-Fock and random-coupling models may be summarized very simply: The only diagrams which survive in the irreducible expansion for $M_k(\zeta_a)$ are those for which the associated ϕ product has the value one for all values of the intermediate momenta allowed by momentum conservation. The contributions of the surviving

diagrams have precisely the same form in the models as in the true problem. This general result is also true for the ring and ladder models under the assumptions of Sec. 5.1. Analysis similar to that we have described shows that the irreducible diagrams in which the ϕ product can exhibit a randomly fluctuating phase give vanishing contributions in the limit $\Omega \rightarrow \infty$. We shall now identify the surviving irreducible diagrams in the ring and ladder models and construct the corresponding closed expressions for $M_k(\zeta_a)$.

It follows from (3.11) and (3.12) that the first three of relations (5.4) are satisfied in the ring model. Thus the irreducible diagrams Figs. 3b, 3c, and 4a survive. However, the ϕ product associated with Fig. 4b is

$$\phi_{kpr s} \phi_{srkp} = \exp \left[i(\bar{\theta}_{ks} + \bar{\theta}_{pr}) + i(\bar{\theta}_{sp} + \bar{\theta}_{rk}) \right]. \quad (5.7)$$

The random phase of this product does not vanish when p, r, and s are constrained by momentum conservation alone. Consequently, the diagram does not survive. The further irreducible diagrams which do survive in the ring model are the infinite class of ring diagrams, whose first two members are shown in Fig. 7. (If the incoming and outgoing external lines are joined together, these diagrams form symmetrical rings.) The ϕ products associated with the successive ring diagrams have the phases

$$\begin{aligned} & \left[(\bar{\theta}_{ks} + \bar{\theta}_{pr}) + (\bar{\theta}_{rp} + \bar{\theta}_{p'r'}) + (\bar{\theta}_{r'p'} + \bar{\theta}_{sk}) \right], \\ & \left[(\bar{\theta}_{ks} + \bar{\theta}_{pr}) + (\bar{\theta}_{rp} + \bar{\theta}_{p'r'}) + (\bar{\theta}_{r'p'} + \bar{\theta}_{p''r''}) + (\bar{\theta}_{r''p''} + \bar{\theta}_{sk}) \right], \\ & \dots \end{aligned} \quad (5.8)$$

which all vanish, by (3.12).

It may be seen from the rules of Sec. 4 that the ring diagrams give a set of contributions to $M_K(\xi_a)$ which resemble a geometric series. They may be summed easily by the usual methods for such series. If we include also the contributions from Figs. 3b, 3c, and 4a, the final result for $M_K(\xi_a)$ is

$$M_K(\xi_a) = \sum_p (V_0 + V_{k-p}) \bar{N}_p + \beta^{-2} \sum_{psbc} V_{k-s} V_{s-k}'(\xi_{c-a}) S_p(\xi_b) S_s(\xi_c) S_{k+p-s}(\xi_{a+b-c}), \quad (5.9)$$

where $V_q'(\xi_d)$ is defined by

$$V_q'(\xi_d) = V_q + \beta^{-1} \sum_{p'b'} V_q S_{p'}(\xi_{b'}) S_{p'-q}(\xi_{b'-d}) V_q'(\xi_d). \quad (5.10)$$

The terms in (5.9) proportional to \bar{N}_p arise from the Hartree-Fock diagrams Figs. 3b and 3c. To verify the remainder of the result, we may solve (5.10) by iteration to yield $V_q'(\xi_d)$ as a function of V_q , and then substitute in (5.9). The zeroth term V_q in the series for $V_q'(\xi_d)$ gives rise to the contribution of Fig. 4a, and the higher terms give the successive ring diagram contributions.

Equation (5.10) may be rewritten

$$V_q'(\xi_d) = V_q \left[1 + \beta^{-1} \sum_{p'b'} V_q S_{p'-q}(\xi_{b'-d}) S_{p'}(\xi_{b'}) \right]^{-1}. \quad (5.11)$$

which vanish identically. The ladder and exchange ladder diagrams exhaust the higher irreducible diagrams which survive in the ladder model. (It should be noted that according to the rules of Sec. 4 diagrams like Fig. 9a and Fig. 9b, which are topologically identical with Figs. 6a and 8b, respectively, are not to be counted separately.)

The contributions of the ladder and exchange ladder diagram sequences can easily be summed in closed form, in a similar fashion to the ring diagrams. If we include also the contributions from Figs. 3b, 3c, 4a, and 4b, the final result for the ladder model is

$$\begin{aligned}
 M_k(\zeta_a) = & \sum_p (V_0 + V_{k-p}) \bar{N}_p \\
 & + \beta^{-2} \sum_{psbc} (V_{k-s} + V_{p-s}) V_{srpk}'(\zeta_{a+b}) S_p(\zeta_b) \\
 & \times S_s(\zeta_c) S_{k+p-s}(\zeta_{a+b-c}), \quad (5.13)
 \end{aligned}$$

where $V_{srpk}'(\zeta_{a+b})$ is defined by

$$\begin{aligned}
 V_{srpk}'(\zeta_{a+b}) = & V_{s-k} - \beta^{-1} \sum_{s'c'} V_{s-s'} V_{s'r'pk}'(\zeta_{a+b}) \\
 & \times S_{s'}(\zeta_{c'}) S_{r'}(\zeta_{a+b-c'}), \quad (5.14)
 \end{aligned}$$

$r = k + p - s$ and

with $\bigwedge r' = k + p - s'$. As in the ring model result, the terms in (5.13) proportional to \bar{N}_p arise from Figs. 3b and 3c. If (5.14) is expanded by iteration and the result for $V_{srpk}'(\zeta_{a+b})$ is substituted in (5.13), the explicit contributions from Figs. 4a, 4b, and the two ladder sequences

are obtained. The non-exchange diagrams all arise from the factor V_{k-s} which appears in (5.13) and the exchange diagrams all arise from the factor \bar{V}_{p-s} when this procedure is carried out. The quantities $V_{srpk}'(\xi_{a+b})$ may be regarded as defining an effective potential for the ladder model.

If the symmetry constraint (3.7) is relaxed in assigning random values to the phases θ_{kp} , an abbreviated ladder model results in which none of the exchange diagrams survive. The abbreviated model violates the second of conditions (3.5), and in consequence it requires an elaboration of our diagram formalism: The two junctions which make up a vertex must be distinguished. We shall not discuss this model further here.

Equations (4.12), (5.9), and (5.10) constitute a closed set of integral equations which determine $S_k(\xi_a)$ for the ring model. Similarly, (4.12), (5.13), and (5.14) constitute a closed set for the ladder model. These equations incorporate extensive classes of terms from the primitive diagram expansion for $S_k(\xi_a)$ in the true problem. They include all primitive diagrams which can be obtained from the surviving irreducible diagrams by repeatedly inserting these irreducible diagrams into themselves and each other as self-energy parts. Examples of complicated primitive diagrams included in the ring and ladder models are shown in Figs. 10a and 10b, respectively.

6. RELATION BETWEEN DISTINGUISHABLE AND INDISTINGUISHABLE PARTICLE MODELS

We wish now to establish a correspondence between the models formulated in Secs. 2 and 3 and thereby verify that the thermodynamic relations

obtained in Sec. 2 are at least formal classical limits for the fermion and boson models. The correspondence is already suggested by the identity of the lower bounds on the ring and ladder model Hamiltonians which we found in the two cases. Our procedure here will be to formulate the distinguishable-particle problem in terms of second-quantized fields, one for each particle. Then we shall appeal to two assumptions: The thermodynamic equivalence of canonical and grand canonical ensembles for infinite systems, and the equivalence of distinguishable and indistinguishable particles in the classical limit.

The Hamiltonian of a system of \bar{N} distinguishable but similar particles interacting through the pair potential $V(x)$ may be written

$$H = \sum_n \sum_k \epsilon_k a_{k(n)}^\dagger a_{k(n)} + H_1, \quad (6.1)$$

$$H_1 = \frac{1}{2} \sum_{nm} \sum_{kprs} V_{k-s} \delta_{k+p, r+s} a_{k(n)}^\dagger a_{p(m)}^\dagger a_{r(m)} a_{s(n)} \quad (6.2)$$

$$(n, m = 1, 2, \dots, \bar{N}).$$

Here we have introduced a separate second-quantized field [labeled (n)] for each particle, and we restrict the system to those states which are eigenstates with eigenvalue one for all the number operators

$$N_{(n)} = \sum_k N_{k(n)} = \sum_k a_{k(n)}^\dagger a_{k(n)}. \quad (6.3)$$

The commutation relations are

$$\left[q_{k(n)}, q_{p(m)}^\dagger \right]_{\pm} = \delta_{nm} \delta_{kp}. \quad (6.4)$$

The restriction of each field to one-particle states makes the choice of plus or minus commutator immaterial.

Let us consider the limit $\bar{N} \rightarrow \infty$ with β and $\rho = \bar{N}/\Omega$ constant. We shall assume in this limit that the canonical ensemble for our system gives the same thermodynamics as a grand canonical ensemble in which all states of the second-quantized fields are admitted. The latter ensemble is chosen so that

$$\langle N_{(n)} \rangle = 1, \quad \langle N \rangle = \sum_n \langle N_{(n)} \rangle = \bar{N}, \quad (6.5)$$

where

$$\langle N_{(n)} \rangle = \text{Tr} \left\{ e^{-\beta(H-\mu N)} N_{(n)} \right\} / \text{Tr} \left\{ e^{-\beta(H-\mu N)} \right\}. \quad (6.6)$$

We should note that (6.5) implies $\mu \rightarrow -\infty$ when $\bar{N} \rightarrow \infty$ with constant ρ and β , as may readily be verified for free particles. The consequence is that the one-particle distribution function takes the Maxwell-Boltzmann form in the limit, as it must for consistency. We may also note that the variance $\langle (N_{(n)} - 1)^2 \rangle$ vanishes in the limit.

Now let us replace (6.2) with a model H_1 ,

$$H_1 = \frac{1}{2} \sum_{nm} \sum_{kprs} v_{k-s} \phi_{kprs} \delta_{k+p, r+s} q_{k(n)}^\dagger q_{p(m)}^\dagger q_{r(m)} q_{s(n)}, \quad (6.7)$$

where the ϕ_{kprs} are the same parameters as in Sec. 3. The thermodynamics

of the model system may be obtained by a propagator formalism very similar to that of Sec. 4. Let us write

$$S_k(u, u') = \sum_n S_{k(n)}(u, u') = - \sum_n \left\langle T \left[q_{k(n)}(u) q_{k(n)}^\dagger(u') \right] \right\rangle, \quad (6.8)$$

and then define $S_k(\xi_a) = \sum_n S_{k(n)}(\xi_a)$ in terms of this $S_k(u, u')$ by (4.6). Again, it will not affect the final results whether the fermion or boson case is taken. With these definitions, we find that (4.8) and (4.10) hold also for the present system, with $N_k \equiv \sum_n N_{k(n)}$. (Of course, for given ρ and β , the chemical potential μ will be very different in the present case than in Sec. 4, as we have noted above.)

Let us write

$$S_{k(n)}^{(0)}(\xi_a) = (\xi_a - \epsilon_k)^{-1}. \quad (6.9)$$

Then the primitive linked-diagram expansion for $S_k(\xi_a)$ is given by the rules of Sec. 4 provided the following changes are made:

a) Give each line a particle label as well as a momentum label.

Associate with each line a factor of the form (6.9).

b) With each vertex, bearing momentum labels p, q, r, s and particle labels n, m, m', n' as shown in Fig. 11, associate a factor

$$-\beta^{-1} \phi_{pqrs} V_{p-s} \delta_{p+q, r+s} \delta_{b+c, d+e} \delta_{nn'} \delta_{mm'}.$$

c) Sum the final result over all values of all the particle labels, including those on the external lines.

The principal difference between the results of this expansion and that of Sec. 4 is that now the contributions of all diagrams with particle exchange vanish in the limit $\bar{N} \rightarrow \infty$, $\Omega \rightarrow \infty$, as we would expect. The formal reason this happens is that the factors of the form δ_{nm} , severely restrict the summations over particle labels in the exchange diagrams. In the diagrams without exchange, each closed loop represents a separate intermediate particle which interacts with the incoming particle or with another intermediate particle. Examples are shown in Fig. 12.

Suppose that we now determine the ϕ_{kprs} by (3.6) and (3.7), the conditions for the fermion or boson ladder model. It is clear from Sec. 5.3 that if similar analysis is carried out for the present case, the surviving diagrams will be all those which arise from the irreducible diagrams Figs. 3b, 4a, and the ladder sequence illustrated in Fig. 6. As we have just noted, there are no exchange contributions for the present system, and consequently the exchange ladder sequence of Fig. 8 gives nothing.

Let us compare this result with what we get from the distinguishable-particle ladder model of Sec. 2. We replace (6.7) by the interaction Hamiltonian

$$H_1 = \frac{1}{2} \sum_{nm} \sum_{kprs} V_{k-s} \phi_{n,m;k-s} \delta_{k+p,r+s} q_{k(n)}^\dagger q_{p(m)}^\dagger q_{r(m)} q_{s(n)}, \quad (6.10)$$

where the $\phi_{n,m;k-s}$ are given by (2.9) et seq. It is clear that the only change in the expansion for $S_K(\zeta_A)$ is that the factor $\phi_{pqrs} V_{p-s}$ in rule b) above must be replaced by the factor $\phi_{n,m;p-s} V_{p-s}$.²² We readily find that

precisely the same diagrams survive in the present case as for the previous ladder model. We shall illustrate the equivalence by two examples.

Consider first the diagram of Fig. 12c and equip it with momentum labels as in Fig. 6a. Its contribution contains the factors

$$V_{k-s} V_{s-s'} V_{s'-k} \exp \left\{ -i \left[(k-s) + (s-s') + (s'-k) \right] \cdot d_{n,m} \right\}, \quad (6.11)$$

according to our rules and to (2.9). The phase of this expression is identically zero, and consequently the contribution survives when it is summed over the particle labels n and m in accord with rule c).

Next, however, consider the ring diagram Fig. 12d, with momentum labels as in Fig. 7a. Its contribution contains the factors

$$V_q V_q V_q \exp \left[-iq \cdot (d_{n,\ell} + d_{\ell,m} + d_{m,n}) \right], \quad (6.12)$$

where $q \equiv k-s$ and we have used the momentum conservation relations. The phase of this expression fluctuates at random as we sum over all values of n , ℓ , and m , so that the contribution does not survive in the limit $\bar{N} \rightarrow \infty$, $\Omega \rightarrow \infty$. (The contribution from the special value $q = 0$ also vanishes in the limit.)

The equivalence of the distinguishable and indistinguishable ring, random-coupling, and Hartree-Fock models may be verified in a similar fashion. We shall give one further illustration: Consider again Fig. 12d, with momentum labels as in Fig. 7a, but now fix the $\phi_{n,m;k}$ by relation (2.19) for the ring model. The contribution from this diagram now contains the factors

$$V_q V_q V_q \exp \left\{ i \left[(\theta_{n;q} + \theta_{l;-q}) + (\theta_{l;q} + \theta_{m;-q}) + (\theta_{m;q} + \theta_{n;-q}) \right] \right\} , \quad (6.15)$$

and we see from (2.20) that the phase vanishes.

We have seen that the thermodynamics of our second-quantized distinguishable-particle system is formally the same in the limit $\bar{N} \rightarrow \infty$, $\Omega \rightarrow \infty$ whether the models of Sec. 2 or those of Sec. 3 are used. Our argument was based on the equivalence of canonical and grand canonical ensembles for the system, and also implicitly made use of assumption 5 of Sec. 5.1, which underlies all our work. Now let us make the further assumption that in the classical limit (sufficiently high temperature and low density) the thermodynamics of fermion, boson, and distinguishable particle systems become identical in the true problem (all ϕ 's = 1), provided the same values of ρ and β are taken in each case. We have seen that, except for exchange diagrams, the models of Sec. 3 select precisely the same diagrams from the true-problem expansion for $S_k(\zeta_a)$ in all three cases: fermion, boson, and distinguishable-particle. However, the exchange diagrams do not contribute in any event in the classical limit. It then follows from all this that the models of Sec. 2, applied to a distinguishable particle system, should give the same thermodynamics in the classical limit as the models of Sec. 3, applied to fermions and bosons. It follows that the classical results of Sec. 2 for A should represent classical limits of the ring, ladder, random-coupling, and Hartree-Fock models for fermions or bosons.

It may also be possible to investigate the relation between our two kinds of models by using the formalisms of Montroll and Ward³ or Lee and Yang²³, neither of which require second-quantization. In the method of Lee and Yang, the thermodynamics of distinguishable (Maxwell-Boltzmann) particles is expressed in terms of a 'binary kernel' which is determined from the ordinary two-particle matrix elements

$$\langle k, p | H_1 | s, r \rangle = V_{k-s} \delta_{k+p, r+s} . \quad (6.14)$$

Then an algorithm is used to obtain results for fermions or bosons. To attempt an expression of our models in this formalism, we would replace (6.14) by the model matrix element

$$\langle k, p | H_1 | s, r \rangle_{n, m} = \phi_{n, m; k-s} V_{k-s} \delta_{k+p, r+s} \quad (6.15)$$

for the Sec. 2 models, or by

$$\langle k, p | H_1 | s, r \rangle_{n, m} = \phi_{kpr s} V_{k-s} \delta_{k+p, r+s} \quad (6.16)$$

for the Sec. 3 models. Here n and m denote the pair of particles for which the matrix element is evaluated. We have not explored this procedure.

Recognition of the thermodynamic results of Sec. 2 as classical limits for the fermion and boson models may provide some useful insights into the behavior of the latter. For example, the lack of saturation found in the classical ladder model suggests that a similar lack characterizes the fermion and boson ladder models. However, the correspondence between the Sec. 2 and Sec. 3 models also leads to a rather discouraging general observation. It points out how modest are the presently feasible

quantum-mechanical diagram summations compared to known classical ones. Our fermion and boson ladder and ring summations, carried out in Sec. 5.3, are more comprehensive than those usually employed; they include infinite classes of self-energy corrections which usually are omitted. Nevertheless, we have seen that the ladder summation corresponds in the classical limit to just one term in the Mayer irreducible cluster expansion. Similarly, our ring summation represents only a partial contribution from each term of the classical irreducible ring diagram sequence. The familiar Montroll-Mayer summation (2.29) appears to correspond, in the quantum-mechanical case, to retaining both ladder and ring summations, together with the self-energy corrections of all orders obtained by repeatedly inserting the retained irreducible diagrams as self-energy parts.

7. DISCUSSION

In the present paper we have obtained formally exact closed equations which express the statistical mechanics of a class of model Hamiltonians for infinite many-body systems. The potential value of these equations lies largely in the fact that certain of the models, the ring and ladder models, share important boundedness properties with the true many-body Hamiltonian: The eigenvalues of the ladder-model Hamiltonian are non-negative if the pair potential $V(x)$ is purely repulsive, and those of the ring-model Hamiltonian are bounded from below if $V(x)$ is bounded and has a non-negative Fourier transform.

These properties suggest that the ring and ladder models, with appropriate $V(x)$, should have a meaningful statistical mechanics even in the zero-temperature limit. Moreover, the structure of the models is such that they embody some important qualitative dynamical features of the true many-body system. For example, we may expect that dissipative damping of single-particle excitations survives in the models. This is particularly clear in the distinguishable-particle formulation of the models: each particle interacts individually with every other particle. A similar situation exists for the fermion and boson models, but there it is more natural to think of interaction among individual momentum modes rather than among individual particles.

The remarks just made suggest that the ladder or ring models may be appropriate for investigating whether the sharp Fermi surface of an infinite system of uncoupled fermions at zero temperature persists when the particles are coupled. Similarly, the model solutions may be of aid in deciding whether singular occupancy of the zero-momentum state, which characterizes an infinite free-boson system at very low temperatures, persists when the particles are coupled. (We anticipate here the extension of our analysis to low-temperature boson systems which will be carried out in the following paper.) The natural way in which the effective density components ρ_k appear in the ring model suggests that it may be appropriate for investigating phonon-like excitations and other collective phenomena.

However, any confidence which our rigorously bounded model Hamiltonians may inspire in a given problem does not automatically extend to

the closed equations which we have derived for the model propagators. First we must establish that these equations are exact descriptions of the models in actuality, as well as formally. This has not been done in the present paper. As we discussed in Sec. 5.1, a fundamental convergence question relating to extremely high-order diagrams is involved. We shall state this question more precisely in Sec. 4 of the following paper, using generalized stochastic models which yield our formally closed equations for finite as well as infinite systems. In Sec. 7 of that paper, we shall outline what we hope is the basis for a satisfying justification of our closed model propagator equations.

The analysis in the following paper is concerned almost exclusively with the indistinguishable-particle models, and we shall not attempt there to offer explicit justification for the assumptions which underlie the classical results of the present Section 2. However, we have already found a degree of support for these results: The closed expressions for the Helmholtz free energy obtained in Sec. 2 reproduced precisely the rigorous lower bounds on the ring and ladder model potential energies.

Our third model, the random-coupling model, exhibited no lower bound on the potential energy per particle in the limit of an infinite system. The results of Sec. 2.4 suggest that this is the case whatever the form of $V(x)$. Consequently, we must expect the random-coupling model not to give sensible statistical-mechanical results at zero temperature in either the classical or the quantum-mechanical case.²⁴

The assured failure of the random-coupling model at zero temperature may point a moral. We have seen in Sec. 5 that this model corresponds to taking just the lowest few diagrams in the irreducible diagram expansion

of the propagator for the true many-body Hamiltonian. The failure of the model suggests that a term-by-term treatment of the irreducible diagram expansion for the true problem may not be justified at very low temperatures, and that results obtained from such a treatment should be viewed with caution.

A general question raised by the present paper is whether there exists an infinite sequence of stochastic models which correspond to more and more comprehensive (but summable) classes of terms from the linked diagram expansion for the true many-body problem. We have so far not succeeded in constructing substantially more elaborate models than those presented here. An obvious next step is to seek a model that combines both ring and ladder summations so as to correspond to the classical Montroll-Mayer ring-diagram summation. On the basis of a preliminary investigation, we offer the following opinion: If such a model can be constructed within the general formal framework of Sec. 3.1, it probably can be achieved only by allowing the parameters ϕ_{kprs} to have stochastically distributed moduli as well as phases.

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APPENDIX

We wish to discuss here two topics which arose in Sec. 2: the derivation of (2.11) for the classical models, and the significance of the condition $(\partial p / \partial \rho)_\beta < 0$ for the models

Equation (2.11) for the true problem usually is derived on the basis of the grand canonical ensemble and rigid-wall boundary conditions. It then is formally exact in the limit $\Omega \rightarrow \infty$. [See, for example, T.L. Hill, Statistical Mechanics (McGraw-Hill Book Company, Inc., New York, 1956), chap. 5.] However, with our cyclic $V(x)$ the factoring of reducible cluster integrals into irreducible integrals is exact for any Ω . Consequently, (2.11) is formally valid for any Ω , with the grand canonical ensemble. In the limit $N \rightarrow \infty$, $\Omega \rightarrow \infty$ it is usually considered immaterial whether the grand canonical or canonical distribution is used, and we shall assume that this is so here.

In the case of our models, a grand canonical ensemble can be formed by considering each of the N particles in the canonical ensemble as a separate species and taking an activity such that the mean total number of particles over the grand ensemble is N . [In doing this, we may extend (2.5) - (2.8) to include the case $n = m$, so as to allow interaction among particles of the same species.] The derivation of (2.11) in the limit $N \rightarrow \infty$, $\Omega \rightarrow \infty$, with B_α interpreted as in the text, then depends upon two facts. First, a reducible cluster integral involving any given $\alpha + 1$ particles factors exactly into irreducible cluster integrals. As in the true problem, this is true for

any α because $V^{n,m}(x)$ is cyclic. Second, if B_α is averaged over all N choices of the species of any one of the particles in the cluster, then (in the limit $N \rightarrow \infty$, $\Omega \rightarrow \infty$) the result is the same for all choices of the species of the other particles, except for a set of choices of relative measure zero. This can be seen for each of the models by analysis similar to that used in the text to evaluate the B_α . We shall not give here a detailed derivation of (2.11) for the models. It is straightforward once the two facts just stated are established.

As in the true problem, we assume in the text that the final averages for an infinite system are independent of whether the grand canonical or canonical ensemble is used. The canonical ensemble is taken in Sec. 2 because it makes the discussion simpler. In the quantum-mechanical treatment of Sec. 6, the grand ensemble is employed.

The derivation and analysis of (2.11) for the models takes a much more elegant form if one uses the generalized models described in Appendix A of reference 11. Then, with the grand ensemble, the formulation in terms of averaged irreducible clusters is exact for all N and Ω .

The statement in the text that $(\partial p / \partial \rho)_\beta < 0$ implies instability must be carefully qualified. Actually, the condition $(\partial p / \partial \rho)_\beta < 0$, or even $p < 0$, does not necessarily imply instability for any of our models, if p is defined as $\rho^2 (\partial A / \partial \rho)_\beta$. This is because of the peculiar way in which the potentials $V^{n,m}(x)$ are constructed. The simplest illustration is provided by the Hartree-Fock model as described by (2.34) and (2.39). Suppose that we have $V_0 < 0$, so that the potential energy per particle (which is just $A-A_0$ for this model) decreases without limit as ρ increases;

that is, as we pack more particles into a fixed volume Ω . By (2.35), we have $p < 0$ and $(\partial p / \partial \rho)_{\beta} < 0$, if ρ is high enough. However, since each particle moves in a uniform potential, the potential energy is independent of configuration, for given N and Ω , and the system is not unstable. Instability arises only if, as we pack the N particles into a closer configuration, we decrease correspondingly the volume of the cyclic cube. Then, since $V_0 \propto \Omega^{-1}$, the potential energy becomes increasingly negative and the system can collapse catastrophically.

It is likely that the relation $(\partial p / \partial \rho)_{\beta} < 0$ has a similar interpretation for all the models treated in this paper. This condition need not imply instability if Ω is fixed, which it must be as we have defined the models. However, if we were to allow Ω to vary in accordance with the actual gross volume occupied by the particles, there would be instability. Having Ω vary would actually be a physically appropriate procedure, as the Hartree-Fock example suggests. For this reason, we consider $(\partial p / \partial \rho)_{\beta} < 0$ to be an instability indication in making a physical interpretation of our models.

It should be noted also that the lack of a lower bound on the potential energy of a system does not preclude a stable thermodynamics. If the density-of-states $\sigma(E)$ (where E is the total energy) decreases faster than exponentially as $E \rightarrow -\infty$, a stable thermal equilibrium can exist for all finite β . If the decrease is slower than exponential, equilibrium will be impossible at any β , while, if the decrease is exponential, equilibrium can exist only if β is less than a critical value.

We wish finally to note the conclusion of L. van Hove [Physica 15, 951 (1949)] that $(\partial p / \partial \rho)_\beta < 0$ cannot be an exact theoretical result for a gas of pair-wise interacting particles. Although it seems assuredly valid for actual physical systems, van Hove's result does not appear to be applicable here. Our models violate an assumption basic to his analysis: The $V^{n,m}(x)$ are defined in such a way that it is not possible to divide the system into effectively non-interacting macroscopic sub-volumes. (Van Hove's result clearly is not valid for the Hartree-Fock example discussed above.) It should be stressed, however, that the results obtained in Sec. 2 are not rigorously justified by the analysis we have presented. As we have noted, there is a fundamental convergence question involved. We shall take up this question in the following paper.

FOOTNOTES

1. One way to obtain this result is the following. Take $\lambda \leq 0$ (pure attractive potential). Then every diagram in the irreducible cluster expansion for pressure gives a negative contribution. The total number of diagrams of order n increases with n faster than any exponential, and a consequence is that the pressure comes out negatively infinite no matter how small $|\lambda|$ is. (Physically, this means the system will collapse.) On the other hand, for $\lambda > 0$, the pressure must approach the perfect gas value as $|\lambda| \rightarrow 0$. Therefore the pressure is a nonanalytic function of λ at $\lambda = 0$. [Cf. T.D. Lee and C.N. Yang, Phys. Rev. 105, 1119 (1957).]
2. T. Matsubara, Progr. Theoret. Phys. (Kyoto), 14, 351 (1955).
3. E.W. Montroll and J.C. Ward, Phys. Fluids 1, 55 (1958).
4. C. Bloch and C. De Dominicis, Nuclear Phys. 7, 459 (1958).
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7. P.C. Martin and J. Schwinger, Phys. Rev. 115, 1342 (1959).
8. J.M. Luttinger and J.C. Ward, Phys. Rev. 118, 1417 (1960).
9. D.N. Zubarev, Usp. Fiz. Nauk. 71, 71 (1960) [translation: Soviet Phys. Uspekhi 3, 320 (1960)].
10. Extensive further bibliography is given in references 7 and 9.

11. R.H. Kraichnan, Report HT-10, Division of Electromagnetic Research, Institute of Mathematical Sciences, New York University (1961, to appear).

12. See the Appendix.

13. As $\beta \rightarrow \infty$, we have $A_0 \rightarrow 0$, and at zero temperature A becomes just the potential energy per particle.

14. The following may make clear how this can happen. Take Ω finite (but $\gg r_0^3$) and place an arbitrarily large number of particles into the cube in any desired positions x_n . Whatever the number of particles, and whatever their positions, it is clear that for every pair n, m there will be many possible choices of $d_{n,m}$ such that $|x_n - x_m - d_{n,m}| > r_0$.

15. This statement must be carefully qualified. See the Appendix for a discussion of the condition $(\partial p / \partial \rho)_\beta < 0$.

16. D. Pines and D. Bohm, Phys. Rev. 85, 338 (1952).

17. E.W. Montroll and J.E. Mayer, J. Chem. Phys. 9, 626 (1941).

18. Our result also resembles (except for the term $\frac{1}{2} \rho \Omega V_0$) the classical limit of a quantum-mechanical ring summation given in reference 3 [Eq. (5.14) of that reference]. However, that summation is based on an activity rather than a density expansion. It corresponds to a sum of pure ring diagrams from the primitive (reducible) classical cluster expansion.

19. Our treatment is based principally upon reference 8, but our notation does not agree completely with that of any of the references cited. (The latter differ substantially among themselves.)

20. See N.M. Hugenholtz and D. Pines, Phys. Rev. 116, 489 (1959).

21. If the vertices and junctions were considered distinguishable, one would obtain, for each of our distinct diagrams, a total of $2^n n!$ diagrams, all of which would give identical contributions to $S_k(\xi_a)$. If one counts these diagrams separately, which we do not do, the contribution per diagram obtained by our rules 1-7 must be multiplied by $1/2^n n!$. The latter procedure is adopted in reference 8.

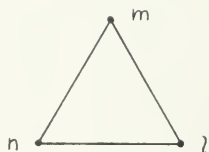
22. We may formally extend the definition of the $\phi_{n,m;k}$ to include the case $n = m$, as we did in Sec. 2.3. This case represents a vanishing contribution here, in the limit $\bar{N} \rightarrow \infty$.

23. T.D. Lee and C.N. Yang, Phys. Rev. 113, 1165 (1959); Phys. Rev. 117, 22 (1960).

24. This does not necessarily exclude the random-coupling model for condensed boson systems. The classical equation of state (2.33) suggests admissibility at any given ρ and β provided $V(x)$ is weak enough. Thus the model may be admissible quantum-mechanically even below the λ -point, if $V(x)$ is weak enough. We regard this argument with strong suspicion.



(a)



(b)



(c)

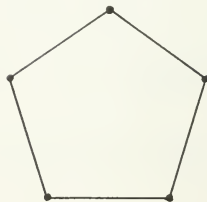
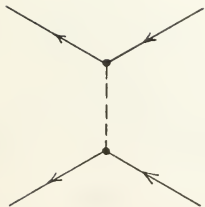
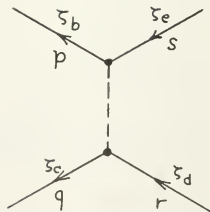


Fig. 1. Some irreducible cluster diagrams.



(a)



(b)

Fig. 2. (a) A vertex. (b) A labeled vertex.

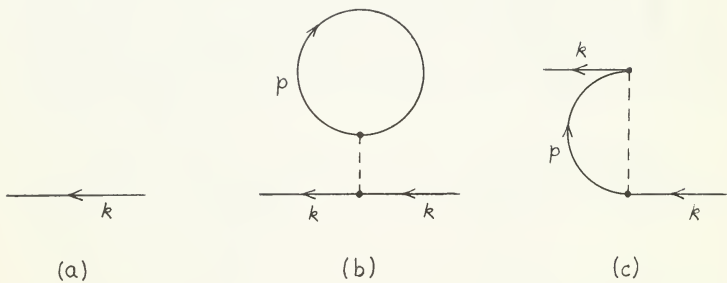


Fig. 3. The zeroth and first-order diagrams for $S_k(\xi)_a$.

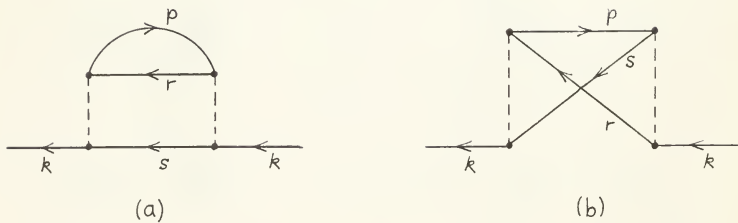


Fig. 4. The second-order irreducible diagrams for $S_k(\xi)_a$.

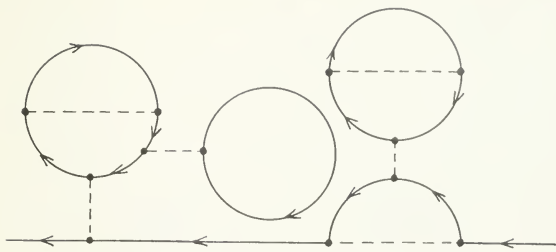


Fig. 5. A primitive diagram which survives in the Hartree-Fock model.

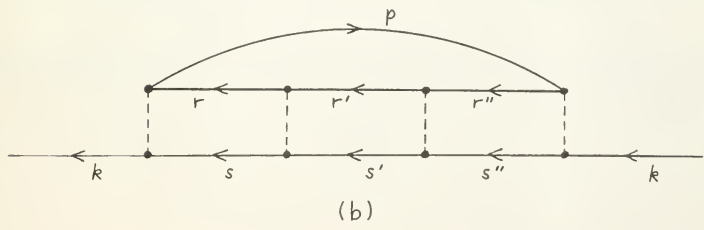
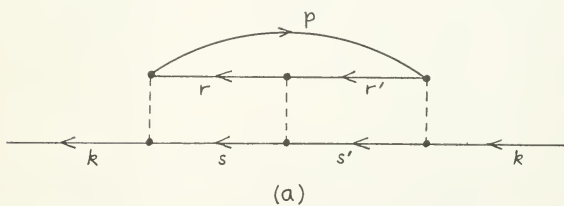


Fig. 6. The third-order and fourth-order ladder diagrams.

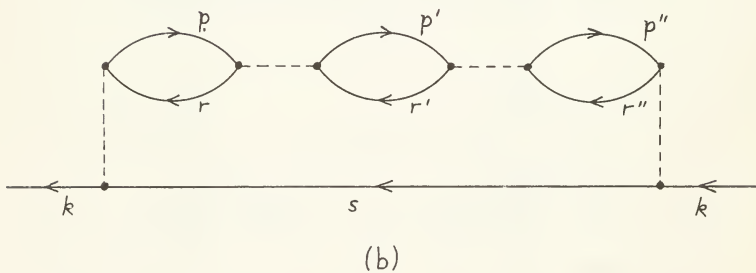
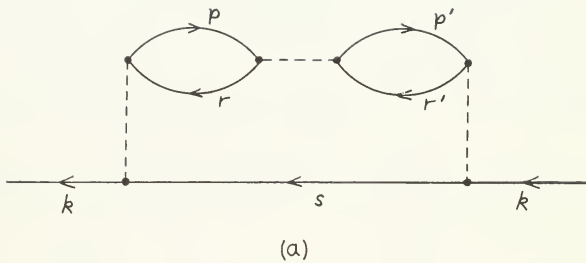
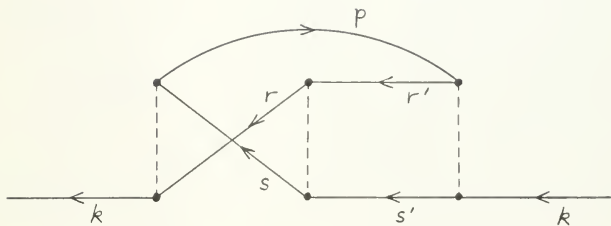
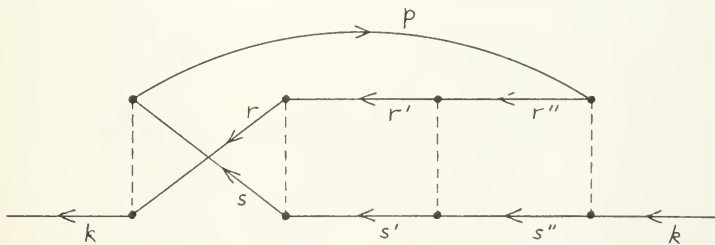


Fig. 7. The third-order and fourth-order ring diagrams.

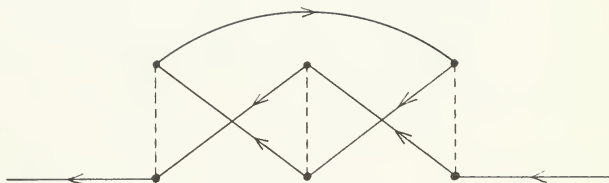


(a)

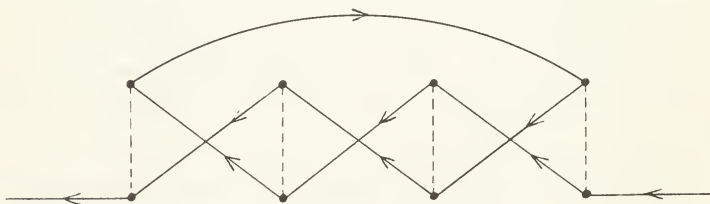


(b)

Fig. 8. The third-order and fourth-order exchange ladder diagrams.



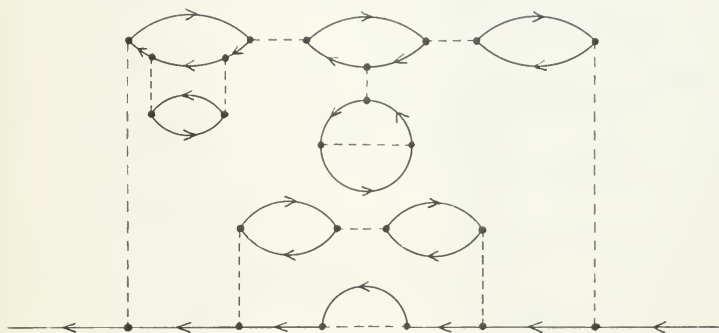
(a)



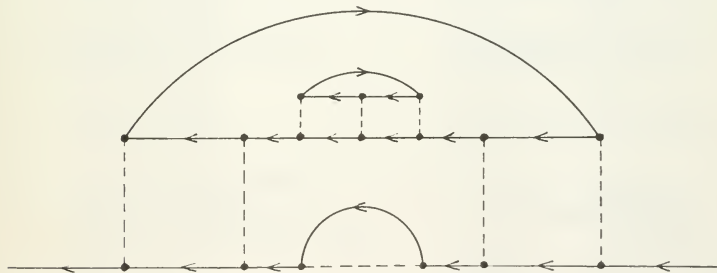
(b)

Fig. 9. (a) A diagram redundant with Fig. 6a.

(b) A diagram redundant with Fig. 8b.



(a)



(b)

Fig. 10. Examples of higher primitive diagrams contributing in the ring model (a) and the ladder model (b).

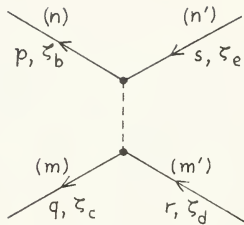


Fig. 11. A labeled vertex for the second-quantized distinguishable particle system.

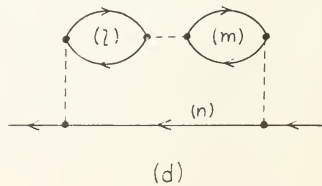
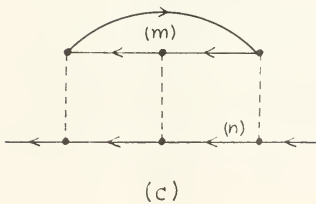
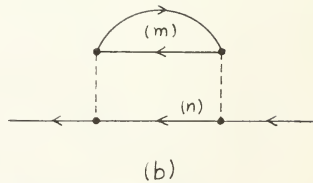
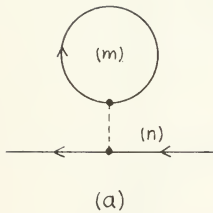


Fig. 12. Some diagrams for the system of distinguishable particles.

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